

Stephen K Gray

List of Publications by Year in descending order

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131
papers

11,786
citations

36303

51
h-index

26613

107
g-index

135
all docs

135
docs citations

135
times ranked

11937
citing authors

#	ARTICLE	IF	CITATIONS
1	Nanostructured Plasmonic Sensors. <i>Chemical Reviews</i> , 2008, 108, 494-521.	47.7	2,245
2	Surface plasmon generation and light transmission by isolated nanoholes and arrays of nanoholes in thin metal films. <i>Optics Express</i> , 2005, 13, 3150.	3.4	466
3	Reversing the size-dependence of surface plasmon resonances. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 14530-14534.	7.1	408
4	Quantum dynamics with real wave packets, including application to three-dimensional $(J=0)D+H_2^+\rightarrow HD+H$ reactive scattering. <i>Journal of Chemical Physics</i> , 1998, 108, 950-962.	3.0	399
5	Quantitative multispectral biosensing and 1D imaging using quasi-3D plasmonic crystals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 17143-17148.	7.1	321
6	Plasmonics in the ultraviolet with the poor metals Al, Ga, In, Sn, Tl, Pb, and Bi. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5415-5423.	2.8	307
7	Near-field dielectric scattering promotes optical absorption by platinum nanoparticles. <i>Nature Photonics</i> , 2016, 10, 473-482.	31.4	298
8	Unimolecular reactions and phase space bottlenecks. <i>Journal of Chemical Physics</i> , 1986, 84, 5389-5411.	3.0	278
9	Nonlocal Optical Response of Metal Nanostructures with Arbitrary Shape. <i>Physical Review Letters</i> , 2009, 103, 097403.	7.8	258
10	Aluminium plasmonics. <i>Journal Physics D: Applied Physics</i> , 2015, 48, 184001.	2.8	218
11	Picosecond energy transfer and multiexciton transfer outpaces Auger recombination in binary CdSe nanoplatelet solids. <i>Nature Materials</i> , 2015, 14, 484-489.	27.5	211
12	Near-Field Photochemical Imaging of Noble Metal Nanostructures. <i>Nano Letters</i> , 2005, 5, 615-619.	9.1	210
13	Propagation of light in metallic nanowire arrays: ϵ -finite-difference time-domain studies of silver cylinders. <i>Physical Review B</i> , 2003, 68, .	3.2	205
14	Excitation of Dark Plasmons in Metal Nanoparticles by a Localized Emitter. <i>Physical Review Letters</i> , 2009, 102, 107401.	7.8	201
15	Quantum-dot-induced transparency in a nanoscale plasmonic resonator. <i>Optics Express</i> , 2010, 18, 23633.	3.4	198
16	Aluminum Nanoparticles as Substrates for Metal-Enhanced Fluorescence in the Ultraviolet for the Label-Free Detection of Biomolecules. <i>Analytical Chemistry</i> , 2009, 81, 1397-1403.	6.5	192
17	Subwavelength light bending by metal slit structures. <i>Optics Express</i> , 2005, 13, 9652.	3.4	185
18	Tailoring the sensing capabilities of nanohole arrays in gold films with Rayleigh anomaly-surface plasmon polaritons. <i>Optics Express</i> , 2007, 15, 18119.	3.4	179

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19	Correlating the Structure, Optical Spectra, and Electrodynamics of Single Silver Nanocubes. <i>Journal of Physical Chemistry C</i> , 2009, 113, 2731-2735.	3.1	171
20	Wave packet dynamics of resonance decay: An iterative equation approach with application to $\text{HCO}^+\text{H}+\text{CO}$. <i>Journal of Chemical Physics</i> , 1992, 96, 6543-6554.	3.0	148
21	Flux analysis for calculating reaction probabilities with real wave packets. <i>Chemical Physics Letters</i> , 1998, 293, 270-276.	2.6	138
22	Symplectic integrators tailored to the time-dependent Schrödinger equation. <i>Journal of Chemical Physics</i> , 1996, 104, 7099-7112.	3.0	134
23	Optical properties of rodlike and bipyramidal gold nanoparticles from three-dimensional computations. <i>Physical Review B</i> , 2007, 76, .	3.2	127
24	Fractal behavior in classical collisional energy transfer. <i>Journal of Chemical Physics</i> , 1986, 84, 2649-2652.	3.0	118
25	Multiscale Model for Photoinduced Molecular Motion in Azo Polymers. <i>ACS Nano</i> , 2009, 3, 1573-1579.	14.6	112
26	Calculating nonlocal optical properties of structures with arbitrary shape. <i>Physical Review B</i> , 2010, 82, .	3.2	112
27	Functional Nanostructured Plasmonic Materials. <i>Advanced Materials</i> , 2010, 22, 1102-1110.	21.0	109
28	Surface Plasmon Standing Waves in Large-Area Subwavelength Hole Arrays. <i>Nano Letters</i> , 2005, 5, 1963-1967.	9.1	100
29	Fragmentation mechanisms from three-dimensional wave packet studies: Vibrational predissociation of NeCl_2 , HeCl_2 , NeICl , and HeICl . <i>Journal of Chemical Physics</i> , 1991, 94, 2817-2832.	3.0	98
30	Wave packet dynamics of van der Waals molecules: Fragmentation of NeCl_2 with three degrees of freedom. <i>Journal of Chemical Physics</i> , 1989, 91, 7671-7684.	3.0	96
31	Quantum dynamics of a planar model for the complex forming $\text{OH}+\text{CO}^+\text{H}+\text{CO}_2$ reaction. <i>Journal of Chemical Physics</i> , 1995, 102, 8807-8817.	3.0	96
32	Probing the effect of the H_2 rotational state in $\text{O}(1\text{D})+\text{H}_2^+\text{OH}+\text{H}$: Theoretical dynamics including nonadiabatic effects and a crossed molecular beam study. <i>Journal of Chemical Physics</i> , 2000, 113, 7330-7344.	3.0	96
33	State-to-state reactive differential cross sections for the $\text{H}+\text{H}_2^+\text{H}_2+\text{H}$ reaction on five different potential energy surfaces employing a new quantum wavepacket computer code: DIFFREALWAVE. <i>Journal of Chemical Physics</i> , 2006, 125, 164303.	3.0	85
34	Apertureless scanning near-field optical microscopy: a comparison between homodyne and heterodyne approaches. <i>Journal of the Optical Society of America B: Optical Physics</i> , 2006, 23, 823.	2.1	80
35	A quantum dynamics study of $\text{H}_2+\text{OH}^+\text{H}_2\text{O}+\text{H}$ employing the Wu-Schatz-Lendvay-Fang-Harding potential function and a four-atom implementation of the real wave packet method. <i>Journal of Chemical Physics</i> , 2002, 117, 1604-1613.	3.0	78
36	Systematic Computational Study of the Effect of Silver Nanoparticle Dimers on the Coupled Emission from Nearby Fluorophores. <i>Journal of Physical Chemistry C</i> , 2008, 112, 11236-11249.	3.1	77

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37	Phase space bottlenecks and statistical theories of isomerization reactions. Journal of Chemical Physics, 1987, 86, 2020-2035.	3.0	75
38	Accurate variational calculations and analysis of the HOCl vibrational energy spectrum. Journal of Chemical Physics, 1998, 109, 10273-10283.	3.0	75
39	Spatial Confinement of Electromagnetic Hot and Cold Spots in Gold Nanocubes. ACS Nano, 2012, 6, 1299-1307.	14.6	75
40	Spectrally Resolved Ultrafast Exciton Transfer in Mixed Perovskite Quantum Wells. Journal of Physical Chemistry Letters, 2019, 10, 419-426.	4.6	74
41	The classical mechanics of vibrational predissociation: A model based study of phase space structure and its influence on fragmentation rates. Journal of Chemical Physics, 1986, 84, 3745-3752.	3.0	73
42	Quantum Wave Packet Study of Nonadiabatic Effects in O(1D) + H ₂ O → OH + H. Journal of Physical Chemistry A, 1999, 103, 9448-9459.	2.5	72
43	Quantum wave packet and quasiclassical trajectory studies of OH+CO: Influence of the reactant channel well on thermal rate constants. Journal of Chemical Physics, 2004, 120, 1231-1238.	3.0	71
44	Plexcitons: The Role of Oscillator Strengths and Spectral Widths in Determining Strong Coupling. ACS Nano, 2018, 12, 402-415.	14.6	71
45	Confining Standing Waves in Optical Corrals. ACS Nano, 2009, 3, 615-620.	14.6	66
46	Size-Dependent Biexciton Quantum Yields and Carrier Dynamics of Quasi-Two-Dimensional Core/Shell Nanoplatelets. ACS Nano, 2017, 11, 9119-9127.	14.6	66
47	Classical Hamiltonian structures in wave packet dynamics. Journal of Chemical Physics, 1994, 100, 5011-5022.	3.0	64
48	Seeing Molecules by Eye: Surface Plasmon Resonance Imaging at Visible Wavelengths with High Spatial Resolution and Submonolayer Sensitivity. Angewandte Chemie - International Edition, 2008, 47, 5013-5017.	13.8	62
49	Ultrafast reversal of a Fano resonance in a plasmon-exciton system. Physical Review B, 2013, 88, .	3.2	62
50	Coriolis induced vibration and rotation mixing in formaldehyde. Journal of Chemical Physics, 1989, 90, 5420-5433.	3.0	54
51	Entanglement of two, three, or four plasmonically coupled quantum dots. Physical Review B, 2015, 92, .	3.2	54
52	Distance Dependence of Förster Resonance Energy Transfer Rates in 2D Perovskite Quantum Wells via Control of Organic Spacer Length. Journal of the American Chemical Society, 2021, 143, 4244-4252.	13.7	54
53	Interfaced Metal Heterodimers in the Quantum Size Regime. Nano Letters, 2013, 13, 3958-3964.	9.1	53
54	Fundamental behavior of electric field enhancements in the gaps between closely spaced nanostructures. Physical Review B, 2011, 83, .	3.2	51

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55	Quantum mechanical calculation of product state distributions for the O(1D)+H ₂ →OH+H reaction on the ground electronic state surface. <i>Journal of Chemical Physics</i> , 2000, 113, 9658-9667.	3.0	50
56	Quantum Mechanical Calculation of Reaction Probabilities and Branching Ratios for the O(1D) + HD → OH(OD) + D(H) Reaction on the X ¹ Σ ⁺ and 11A ¹ Adiabatic Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2001, 105, 2330-2339.	2.5	50
57	Quantum dynamics of ArI ₂ vibrational predissociation including low total angular momenta: The role of intramolecular vibrational energy redistribution. <i>Journal of Chemical Physics</i> , 1996, 104, 4999-5011.	3.0	48
58	Computational study of fluorescence scattering by silver nanoparticles. <i>Journal of the Optical Society of America B: Optical Physics</i> , 2007, 24, 2259.	2.1	47
59	Near-Field Polarization Effects in Molecular-Motion-Induced Photochemical Imaging. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4111-4116.	3.1	47
60	SERS enhancements via periodic arrays of gold nanoparticles on silver film structures. <i>Optics Express</i> , 2009, 17, 8669.	3.4	47
61	Dispersion fitted finite difference method with applications to molecular quantum mechanics. <i>Journal of Chemical Physics</i> , 2001, 115, 8331-8344.	3.0	44
62	DIFFREALWAVE: A parallel real wavepacket code for the quantum mechanical calculation of reactive state-to-state differential cross sections in atom plus diatom collisions. <i>Computer Physics Communications</i> , 2008, 179, 569-578.	7.5	43
63	Rotation-vibration interactions in formaldehyde: Results for low vibrational excitations. <i>Journal of Chemical Physics</i> , 1991, 94, 195-207.	3.0	42
64	Sinc wave packets: New form of wave packet for time-dependent quantum mechanical reactive scattering calculations. <i>International Journal of Quantum Chemistry</i> , 2003, 92, 205-211.	2.0	42
65	Quantum dynamics of van der Waals clusters: Model results for He ₂ Cl ₂ and Ne ₂ Cl ₂ fragmentation. <i>Journal of Chemical Physics</i> , 1993, 98, 5396-5407.	3.0	41
66	Symplectic integrators for the multichannel Schrödinger equation. <i>Journal of Chemical Physics</i> , 1995, 102, 9214-9227.	3.0	41
67	Mapping the Electromagnetic Near-Field Enhancements of Gold Nanocubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 24734-24740.	3.1	41
68	Quantum States of Molecular Hydrogen and Its Isotopes in Single-Walled Carbon Nanotubes. <i>Journal of Physical Chemistry B</i> , 2003, 107, 12989-12995.	2.6	40
69	Surface Plasmon-Enhanced Spectroscopy and Photochemistry. <i>Plasmonics</i> , 2007, 2, 143-146.	3.4	40
70	Surface chemistry: a non-negligible parameter in determining optical properties of small colloidal metal nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11814.	2.8	40
71	A periodically forced oscillator model of van der Waals fragmentation: Classical and quantum dynamics. <i>Journal of Chemical Physics</i> , 1987, 87, 2051-2061.	3.0	39
72	Multispectral Thin Film Biosensing and Quantitative Imaging Using 3D Plasmonic Crystals. <i>Analytical Chemistry</i> , 2009, 81, 5980-5989.	6.5	39

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73	Quantum reactive scattering calculations of cross sections and rate constants for the $N(2D)+O_2(X^3\Sigma_g^-) \rightarrow O(3P)+NO(X^2\Pi)$ reaction. <i>Journal of Chemical Physics</i> , 2003, 118, 3111-3123.	3.0	38
74	Quantum and quasiclassical reactive scattering of $O(1D)+HCl$ using an ab initio potential. <i>Chemical Physics Letters</i> , 1999, 315, 275-281.	2.6	36
75	Time dependent quantum dynamics study of the $O++H_2(v=0,j=0) \rightarrow OH++H$ ion-molecule reaction and isotopic variants (D ₂ ,HD). <i>Journal of Chemical Physics</i> , 2006, 125, 164305.	3.0	36
76	Molded plasmonic crystals for detecting and spatially imaging surface bound species by surface-enhanced Raman scattering. <i>Applied Physics Letters</i> , 2009, 94, 243109.	3.3	36
77	Controlling Plasmonic Wave Packets in Silver Nanowires. <i>Nano Letters</i> , 2010, 10, 3389-3394.	9.1	36
78	Optimization of 3D Plasmonic Crystal Structures for Refractive Index Sensing. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10493-10499.	3.1	34
79	Theory and Modeling of Plasmonic Structures. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1983-1994.	3.1	34
80	Nonlocal Dielectric Effects in Core-Shell Nanowires. <i>Journal of Physical Chemistry C</i> , 2010, 114, 15903-15908.	3.1	33
81	A comparative study of the quantum dynamics and rate constants of the $O(3P)+HCl$ reaction described by two potential surfaces. <i>Journal of Chemical Physics</i> , 2000, 113, 227-236.	3.0	31
82	Wave Packet Calculation of Cross Sections, Product State Distributions, and Branching Ratios for the $O(1D) + HCl$ Reaction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 5743-5750.	2.5	30
83	Soft Embossing of Nanoscale Optical and Plasmonic Structures in Glass. <i>ACS Nano</i> , 2011, 5, 5763-5774.	14.6	30
84	Origins and optimization of entanglement in plasmonically coupled quantum dots. <i>Physical Review A</i> , 2016, 94, .	2.5	30
85	High-Fidelity Nano-Hole-Enhanced Raman Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2009, 113, 11190-11197.	3.1	29
86	The effect of angular momentum on the unimolecular dissociation $HCO \rightarrow H+CO$. <i>Journal of Chemical Physics</i> , 1997, 107, 7773-7786.	3.0	28
87	Optical Scattering from Isolated Metal Nanoparticles and Arrays. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14191-14198.	2.6	28
88	Chemical Reactivity within Carbon Nanotubes: A Quantum Mechanical Study of the $D + H_2 \rightarrow HD + H$ Reaction. <i>Journal of Physical Chemistry C</i> , 2008, 112, 2654-2659.	3.1	28
89	Highly Excited Bound and Low-Lying Resonance States of H_2O . <i>Journal of Physical Chemistry A</i> , 2001, 105, 2634-2641.	2.5	27
90	Theory and modeling of light interactions with metallic nanostructures. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 323201.	1.8	26

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91	On the Feasibility of Using the Intrinsic Fluorescence of Nucleotides for DNA Sequencing. Journal of Physical Chemistry C, 2010, 114, 7448-7461.	3.1	25
92	A scattering resonance description of very low energy collision induced vibrational relaxation. Journal of Chemical Physics, 1985, 83, 2818-2828.	3.0	23
93	Quantum dynamics study of the dissociative photodetachment of HOCO ⁺ . Journal of Chemical Physics, 2006, 125, 164312.	3.0	23
94	Substrate effects on surface plasmons in single nanoholes. Chemical Physics Letters, 2007, 435, 123-126.	2.6	22
95	Plasmonic Electromagnetic Hot Spots Temporally Addressed by Photoinduced Molecular Displacement. Journal of Physical Chemistry A, 2009, 113, 4647-4651.	2.5	22
96	Plasmon-based photopolymerization: near-field probing, advanced photonic nanostructures and nanophotochemistry. Journal of Optics (United Kingdom), 2014, 16, 114002.	2.2	21
97	Enhancing surface plasmon polariton propagation lengths via coupling to asymmetric waveguide structures. Physical Review B, 2008, 77, .	3.2	20
98	Reversible Modulation of Surface Plasmons in Gold Nanoparticles Enabled by Surface Redox Chemistry. Angewandte Chemie - International Edition, 2015, 54, 8948-8951.	13.8	20
99	Reactive scattering. Computer Physics Communications	7.5	19
100	Inhomogeneous Surface Plasmon Polaritons. ACS Photonics, 2014, 1, 739-745.	6.6	19
101	A Quantum Dynamics Study of D ₂ + OH → DOH + D on the WSLFH Potential Energy Function. Journal of Physical Chemistry A, 2003, 107, 7132-7137.	2.5	18
102	Intramolecular and Fragmentation Dynamics of Van der Waals Complexes. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1988, 92, 236-242.	0.9	17
103	Wave packet dynamics of the N(4S)+O ₂ (X ³ Σ ⁻ g ⁻) → NO(X ² Σ ⁺) + O(3P) reaction on the X ² A ² potential energy surface. Journal of Chemical Physics, 2001, 115, 3208-3214.	3.0	17
104	Quantum dynamics of vibrationally activated OH → CO reactant complexes. Journal of Chemical Physics, 2004, 121, 823-828.	3.0	17
105	Theoretical Study of the Complex-Forming CH + H ₂ → CH ₂ + H Reaction. Journal of Physical Chemistry A, 2006, 110, 5542-5548.	2.5	16
106	A transition state real wave packet approach for obtaining the cumulative reaction probability. Journal of Chemical Physics, 2000, 112, 2623-2633.	3.0	14
107	An OpenMP/MPI approach to the parallelization of iterative four-atom quantum mechanics. Computer Physics Communications, 2005, 166, 94-108.	7.5	14
108	Remote grating-assisted excitation of narrow-band surface plasmons. Optics Express, 2010, 18, 23857.	3.4	14

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109	Tailoring the parameters of nanohole arrays in gold films for sensing applications. Proceedings of SPIE, 2007, 6641, 9.	0.8	12
110	THE EQUILIBRIUM CONSTANTS FOR MOLECULAR HYDROGEN ADSORPTION IN CARBON NANOTUBES BASED ON ITERATIVELY DETERMINED NANO-CONFINED BOUND STATES. Journal of Theoretical and Computational Chemistry, 2003, 02, 621-625.	1.8	11
111	Self-Consistent Model of Light-Induced Molecular Motion Around Metallic Nanostructures. Journal of Physical Chemistry Letters, 2010, 1, 2228-2232.	4.6	11
112	Heterodyne apertureless near-field scanning optical microscopy on periodic gold nanowells. Optics Express, 2007, 15, 4098.	3.4	10
113	Theoretical study of the potential energy surfaces and bound states of HCP. Journal of Chemical Physics, 2000, 112, 5866-5876.	3.0	9
114	Multigrid FDTD with Chombo. Computer Physics Communications, 2007, 176, 109-120.	7.5	8
115	Dephasing of electromagnetic fields in scattering from an isolated slit in a gold film. Proceedings of SPIE, 2008, , .	0.8	8
116	Classical Trajectory Studies of the $D + H_2 \rightarrow HD + H$ Reaction Confined in Carbon Nanotubes: Parallel Trajectories. Journal of Physical Chemistry C, 2008, 112, 15260-15266.	3.1	7
117	Quantum dynamics study of the $K + HF(v=0, j=0) \rightarrow KF + H$ reaction and comparison with quasiclassical trajectory results. Journal of Chemical Physics, 2008, 128, 144302.	3.0	7
118	Surrogate-Based Modeling of the Optical Response of Metallic Nanostructures. Journal of Physical Chemistry C, 2010, 114, 20741-20748.	3.1	7
119	Bi-fidelity fitting and optimization. Journal of Chemical Physics, 2012, 136, 074102.	3.0	7
120	Exciton size and quantum transport in nanoplatelets. Journal of Chemical Physics, 2015, 143, 224106.	3.0	5
121	Quantum Mechanical Capture/Phase Space Theory Calculation of the Rate Constants for the Complex-Forming $CH + H_2$ Reaction. Journal of Physical Chemistry A, 2008, 112, 12588-12596.	2.5	4
122	Refractive index sensing and surface-enhanced Raman spectroscopy using silver-gold layered bimetallic plasmonic crystals. Beilstein Journal of Nanotechnology, 2017, 8, 2492-2503.	2.8	4
123	A new expression for the direct quantum mechanical evaluation of the thermal rate constant. Journal of Chemical Physics, 2004, 120, 9060-9070.	3.0	3
124	The use of aluminum nanostructures as platforms for metal enhanced fluorescence of the intrinsic emission of biomolecules in the ultra-violet. Proceedings of SPIE, 2010, 7577, 757700.	0.8	3
125	Orientational Interpolation of the Optical Spectra of Nonspherical Nanoparticles. Journal of Physical Chemistry C, 2012, 116, 12712-12724.	3.1	3
126	Computer science and mathematics for chemistry-related applications. Journal of Mathematical Chemistry, 2012, 50, 379-380.	1.5	3

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127	CHEMICAL REACTION DYNAMICS WITH REAL WAVE PACKETS. Journal of Theoretical and Computational Chemistry, 2002, 01, 373-379.	1.8	1
128	Functional Nanoimprinted Plasmonic Crystals for Chemical Sensing and Imaging. , 2012, , 199-227.		1
129	Classical Dynamics of Van der Waals Molecules. NATO ASI Series Series B: Physics, 1990, , 81-90.	0.2	1
130	Optical near-field enhancement around lithographic metallic nanostructures using an azo-dye polymer: direct observation and realization of sub-wavelength complex structures. Materials Research Society Symposia Proceedings, 2004, 838, 187.	0.1	0
131	RADICAL CHEMISTRY WITH WAVE PACKETS. Advanced Series in Physical Chemistry, 1996, , 504-535.	1.5	0